A molecular-level coupling model of fluid catalytic cracking and hydrotreating processes to improve gasoline quality

Xinglong Qin[1], Lei Ye[2], Alqubati Murad[2], Jichang Liu[1], Qiang Ying[2], Haitao Shen[1], Wenxin Yu[2], Jinquan Xie[2], Lixin Hou[2], Xin Pu[2], Xin Han[2], Jiangbing Li[3], Rongjie Wang [3], and Ning Liu[3]

[1]East China University of Science and Technology School of Chemical Engineering
[2]East China University of Science and Technology
[3]Shihezi University School of Chemistry and Chemical Engineering

May 12, 2022

Abstract

A molecular-level Fluid Catalytic Cracking (FCC)-Gasoline Hydrotreating (GH) process coupling model was established based on the Structure Oriented Lumping (SOL) method to guide the precise control of the hydrocarbon compositions in gasoline. 96 FCC reaction rules and 24 GH reaction rules were formulated, and a reaction network containing about 120,000 reactions was constructed. In order to establish the FCC-GH process coupling model, the effective transfer of composition information between the two processes was realized through the molecular composition matrix of gasoline. The molecular composition matrix of gasoline was obtained according to the classification rules of the molecular composition matrix of FCC products. The conversion laws of hydrocarbon molecules in gasoline were investigated by tracking their generation paths and reaction paths. The influences of reaction conditions on the distribution of hydrocarbons in the product gasoline could be calculated quantitatively by the FCC-GH process coupling model at molecular level.

Hosted file

`Main Document.docx` available at https://authorea.com/users/482368/articles/568959-a-molecular-level-coupling-model-of-fluid-catalytic-cracking-and-hydrotreating-processes-to-improve-gasoline-quality